Novel Carbon-Carbon Nanocomposites: Building 2D and 3D single-walled carbon nanotube Networks

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Due to the remarkable electronic and mechanical properties of single-walled carbon nanotubes (SWNT), various applications for these in nanoscale devices have been described [1]. However, little progress has been reported on techniques related to connecting such tubular structures. The latter is a key issue because both electronic devices and strong nano-mechanical systems need the establishment of molecular connections among SWNTs. In particular, theory predicts that a “Y” or a “T” junction could act as multi-terminal electronic device involving SWNTs [2-4]. Therefore, it is imperative to join and connect nanotubes in a controllable way, however no experiment to date has shown that this proposition is indeed viable. Here, we demonstrate for the first time, that irradiation exposure at elevated temperatures, can be used as an effective tool to covalently weld SWNTs in order to create molecular junctions of various geometries. We have fabricated “Y”, “X” and “T-like” junctions (Fig. 1), that are stable [5]. Tight binding molecular dynamics calculations demonstrate that vacancies, formed under the electron beam, trigger the formation of molecular junctions involving seven or eight membered carbon rings (Fig. 2). Local density of states (LDOS) of junction models, resembling those observed in our experiments, are also described. We envisage that our results will pave the way towards controlled fabrication of nanotube based molecular circuits, nanotube fabrics and network architectures exhibiting exciting electronic and mechanical behaviour.

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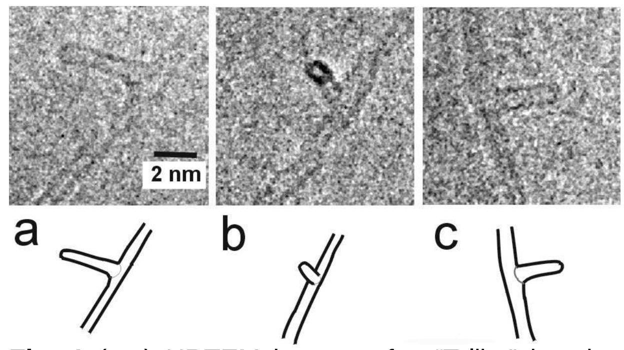

Fig. 1 (a-c) HRTEM images of a “T-like” junction formed after irradiating a “Y” junction. It is possible to thin one of the tubes of the “Y” junction, which eventually breaks and forms a “hook” (not shown here). It is possible to observe the evolution of this junction during irradiation and the rotation by 180° under the electron beam; note the circular cross-section in one of the tubes (b).

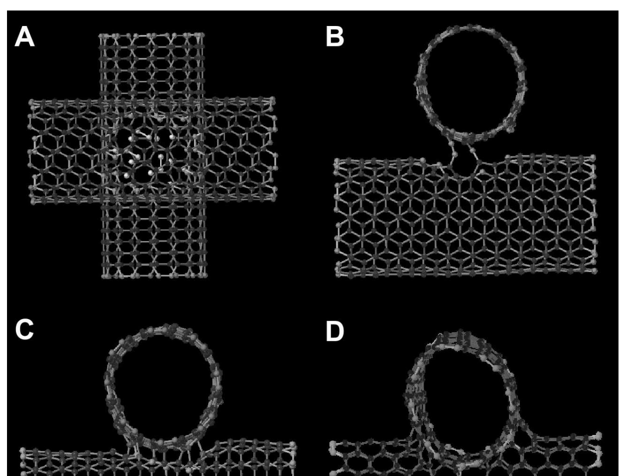

Fig. 2 TBMD simulations at 1000 °C of two crossing (8,8) nanotubes, which transform into an “X” junction: **(a)** Two crossing tubes containing 20 vacancies on their surfaces (top view). The unit cell contains 860 carbon atoms (white, yellow, green, blue and red spheres, illustrating an atomic coordination of 0, 1, 2, 3, and 4, respectively); **(b)** After 10ps, two links between the two defected carbon structures are formed via carbon chains (side view); **(c)** After 100 ps, a surface reconstruction occurs and the resulting structure consists of a molecular “X” junction. This reconstructed surface mainly contains sp^2 carbon atoms, and exhibit six heptagons, one octagon, one pentagon and two dangling bonds. **(d)** After 220ps, a surface reconstruction occurs and the resulting structure consists of a molecular “X” junction. This reconstructed surface mainly contains sp^2 carbon atoms, and exhibit six heptagons, one octagon, one pentagon and two dangling bonds.